

Phthalic acid, 2,2-dichloroethyl isobutyl ester

Inchi:	InChI=1S/C14H16Cl2O4/c1-9(2)7-19-13(17)10-5-3-4-6-11(10)14(18)20-8-12(15)16/h3-6,
InchiKey:	NUFGOHVIMDAQNI-UHFFFAOYSA-N
Formula:	C14H16Cl2O4
SMILES:	CC(C)COC(=O)c1ccccc1C(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	319.18

Physical Properties

Property code	Value	Unit	Source
gf	-326.80	kJ/mol	Joback Method
hf	-638.87	kJ/mol	Joback Method
hfus	32.59	kJ/mol	Joback Method
hvap	76.00	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	3.460		Crippen Method
mcvol	223.720	ml/mol	McGowan Method
pc	2043.76	kPa	Joback Method
rinsol	2056.00		NIST Webbook
tb	777.94	K	Joback Method
tc	997.29	K	Joback Method
tf	460.64	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.47	J/molxK	777.94	Joback Method
cpg	604.08	J/molxK	814.50	Joback Method
cpg	615.67	J/molxK	851.06	Joback Method
cpg	626.26	J/molxK	887.61	Joback Method
cpg	635.86	J/molxK	924.17	Joback Method
cpg	644.49	J/molxK	960.73	Joback Method
cpg	652.16	J/molxK	997.29	Joback Method
dvisc	0.0009319	Paxs	460.64	Joback Method
dvisc	0.0005022	Paxs	513.52	Joback Method

dvisc	0.0003037	Paxs	566.41	Joback Method
dvisc	0.0002002	Paxs	619.29	Joback Method
dvisc	0.0001409	Paxs	672.17	Joback Method
dvisc	0.0001043	Paxs	725.06	Joback Method
dvisc	0.0000805	Paxs	777.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356925&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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